8.0 CONTAMINANT FATE AND TRANSPORT ANALYSIS

An evaluation of the environmental fate and transport of site-related contaminants is important in determining the potential for exposure to the contaminants. There are several mechanisms by which contaminants may migrate at the TP Site. Migration into the air can occur via volatilization or dust generation. Migration into groundwater can occur by percolation of infiltrating rainwater or groundwater flow through waste materials or contaminated soils. Transport to streams in the area can occur via surface water runoff and through groundwater discharge. The mechanisms of migration for the contaminants of concern detected at the site (see Section 9.1.5) are discussed in more detail below. Estimates of the physical and chemical properties of the contaminants of concern which may affect contaminant migration are presented in **Table 8-1**. The general persistence of the contaminants of concern is also discussed below.

8.1 CONTAMINANT MIGRATION

8.1.1 AIR MIGRATION

Generally, volatilization from soil and/or water into air may be an important transport mechanism for the organic chemicals with Henry's Law Constants greater than 10⁻⁵ atm-m³/mole and molecular weights less than 200 g/mole. All of the volatile organic and some of the semi-volatile organic contaminants of concern found at the site meet these criteria, and thus, if subsurface soil and/or groundwater is brought to the surface, volatilization of these contaminants of concern could be an important release mechanism.

Fugitive dust emissions from wind or mechanical disturbances may occur from unpaved or unvegetated areas of the site. The environmental factors that influence wind erosion are wind speed, moisture content, vegetative cover, and soil composition. Because the environmental

TABLE 8-1
ESTIMATED PHYSICAL AND CHEMICAL PROPERTIES OF THE CONTAMINANTS OF CONCERN TENNESSEE PRODUCTS SITE CHATTANOOGA, TENNESSEE

Contaminant of Concern	Molecular Weight (g/mol)	Solubility at 25° C (mg/l)	Henry's Constant (atm-m³/mol x 10 ⁻⁵)	$ m K_{oc}$ (ml/g)	$ m K_{ow} \ (ml/g)$	K_d (ml/g)
	(g/11101 <i>)</i>	(mg/ <i>t)</i>	(aun-in /inoi x 10)		(m/g)	(1111/5)
<u>Inorganics</u>						
Arsenic	NA	NA	NA	NA	NA	200^{4}
Aluminum	NA	NA	NA	NA	NA	
Barium	NA	NA	NA	NA	NA	0.5^{4}
Beryllium	NA	NA	NA	NA	NA	1300^{4}
Cadmium	NA	NA	NA	NA	NA	560^{4}
Iron	NA	NA	NA	NA	NA	170^{4}
Manganese	NA	NA	NA	NA	NA	180^{4}
Nickel	NA	NA	NA	NA	NA	650^{4}
Vanadium	NA	NA	NA	NA	NA	
Cyanide	NA	NA	NA	NA	NA	
<u>VOCs</u>						
Acetone	58^{1}	1000000^{1}	4^1	0.4^{1}	0.6^{1}	0.00045^3
Benzene	78^{1}	1800^{2}	550^{1}	83¹	140^{2}	0.11^{3}
Carbon Tetrachloride	154^{1}	800^{2}	3000^{1}	220^{1}	440^{2}	0.33^{3}
Chlorobenzene113 ¹		470^{2}	390^{1}	330^{1}	690^{2}	0.52^{3}
Chloroform	119^{1}	9600^{2}	340^{1}	44^{1}	93^{2}	0.070^{3}

ESTIMATED PHYSICAL AND CHEMICAL PROPERTIES OF THE CONTAMINANTS OF CONCERN TENNESSEE PRODUCTS SITE CHATTANOOGA, TENNESSEE

TABLE 8-1 (cont.)

of	Molecular Weight (g/mol)	Solubility at 25° C (mg/l)	Henry's Constant (atm-m³/mol x 10 ⁻⁵)	K_{oc} (ml/g)	${ m K}_{ m ow} \ ({ m m} l/{ m g})$	$ m K_d \ (ml/g)$
Ethylbenzene	106^{1}	210^{2}	640^{1}	260^{1}	1400^{2}	1.1^{3}
Methyl Butyl Ketone	100^{1}	$35,000^{1}$	180^{1}	140^{1}	24^{1}	0.018^{3}
Tetrachloroethene	166^{1}	150^{2}	290^{1}	360^{1}	760^{2}	0.57^{3}
Toluene	92^{1}	540^{2}	670^{1}	150^{1}	490^{2}	0.37^{3}
1,1,1-Trichloroethane	133¹	950^{2}	1600^{1}	100^{1}	150^{2}	0.11^{3}
Trichloroethene	1311	1100^{2}	1200^{1}	110^{1}	200^{2}	0.15^{3}
<u>SVOCs</u>						
Benzo(a)anthracene	228^{1}	0.014^{2}	0.066^{1}	1400000¹	140000^2	110^{3}
Benzo(b &/or k)fluoranthene	252^{1}	0.00055^2	1.2^{1}	550000^{1}	3700000^2	2800^{3}
Benzo-a-pyrene	252^{1}	0.0038^2	0.24^{1}	400000^{1}	1100000^2	830^{3}
Bis(2-ethylhexyl)phthalate	391¹	0.4^{2}	1.1^{1}	100000^{1}	540000000^2	410000^3
Carbazole	167^{5}	1.8^{5}	0.0086^{5}	640^{5}	5200^{5}	3.9^{3}
Dibenzo(a,h)anthracene	278^{1}	0.0005^2	0.00073^{1}	1700000^{1}	930000^2	700^{3}
Dibenzofuran	168^{1}	10^{1}	9.7^{5}	10000^{1}	15000^{1}	11^{3}
1,4-Dichlorobenzene	147^{1}	79^{2}	270^{1}	160^{1}	2400^{2}	1.8^{3}
2,4-Dimethylphenol	122^{1}	17000^2	0.66^{1}	120^{1}	320^{2}	0.24^{3}
Indeno(1,2,3-cd)pyrene	276^{1}	0.62^{2}	3000^{1}	31000000^{1}	46000000^2	35000^{3}

TABLE 8-1 (cont.)

ESTIMATED PHYSICAL AND CHEMICAL PROPERTIES OF THE CONTAMINANTS OF CONCERN TENNESSEE PRODUCTS SITE CHATTANOOGA, TENNESSEE

Contaminant of	Molecular Weight	Solubility at 25° C	Henry's Constant	K_{oc}	\mathbf{K}_{ow}	\mathbf{K}_{d}
Concern	(g/mol)	(mg/l)	$(atm-m^3/mol \times 10^{-5})$	(ml/g)	(ml/g)	(ml/g)
2-Methylnaphthalene	142¹	251	52 ⁵	8500¹	13000¹	9.8^{3}
2-Methylphenol	108^{1}	25000^{1}	0.12^{1}	22^{1}	89^{1}	0.067^{3}
3-and/or 4-)Methylphenol	108^{1}	$23,000^{1}$	0.079^{1}	49^{1}	831	0.063^{3}
Naphthalene	128^{1}	34^{2}	48^{1}	1300^{1}	2300^{2}	1.7^{3}
Phenanthrene	1781	1.3^{2}	3.9^{1}	23000^{1}	29000^{2}	22^{3}
Pesticides/PCBs						
Alpha-BHC	2911	2.0^{2}	0.53^{1}	1900¹	6500^{2}	4.9^{3}
Beta-BHC	2911	0.24^{2}	0.023^{1}	2900^{1}	6300^{2}	4.8^{3}
Delta-BHC	291^{1}	31^{2}	0.025^{1}	1900^{1}	14000^2	11^{3}
Dieldrin	3811	0.2^{2}	0.020^{1}	36000^{1}	140000^{1}	110^{3}
PCB-1248	288^{1}	0.054^{2}	350^{1}	440000^{1}	560000^{2}	420^{3}

Notes:

 K_{oc} - Organic carbon partition coefficient

 $K_{\rm ow}$ - Octanol/water partition coefficient

 K_d - Soil/water partition coefficient

NA - Not Applicable

-- - No Data Available

TABLE 8-1 (cont.)

ESTIMATED PHYSICAL AND CHEMICAL PROPERTIES OF THE CONTAMINANTS OF CONCERN TENNESSEE PRODUCTS SITE CHATTANOOGA, TENNESSEE

Sources:

- 1) Montgomery and Welkom (1990)
- 2) Walton (1984)
- Based on the average fraction of organic carbon measured in ten field samples (see Appendix E.4) and the following equation (Walton, 1984):

$$K_d = 0.63 * f_{oc} * K_{ow}$$

 f_{oc} = fraction of organic carbon in soil (0.0012)

- 4) Based on data presented in Thibault, et al. (1990)
- 5) Hazardous Substance Data Bank maintained by the National Library of Medicine in Bethesda, Maryland

factors at the TP Site are at times and places conducive to wind erosion, each of the contaminants of concern detected in surface soil is susceptible to migration via fugitive dust generation.

8.1.2 SURFACE WATER MIGRATION

Contaminant migration into surface waters at the TP Site may occur through surface water runoff and/or through groundwater discharge. Upon reaching surface water, the contaminants may remain in the water column, volatilize, or sorb to bottom or suspended sediments. Volatile organic contaminants tend to quickly volatilize into the atmosphere upon reaching surface water and for this reason are rarely observed at detectable concentrations in surface water samples. Nevertheless, it should be noted that a few volatile organic chemicals were detected at low concentrations in both surface water and sediment samples collected at the site (primarily in the Northeast Tributary). The semi-volatile organics with low water solubilities and high K_{oc} values such as the PAHs, pesticides, and PCBs will tend to associate with sediments. The semi-volatile organics with high water solubilities and low K_{oc} values such as the phenols will tend to stay in the water column. Based on the surface water and sediment sample results obtained in this remedial investigation, it appears that the semi-volatile organics found in the surface waters at the site are primarily PAHs and pesticides, and they appear to be mostly sorbing to sediment particles, as expected.

The behavior of the inorganic contaminants of concern in surface water is affected by pH, temperature, and hardness. Inorganic compounds can occur in aquatic systems as dissolved ions, dissolved complexes with organic and inorganic chemicals, colloids, or particulates. The solubility and mobility of the metal inorganic contaminants is enhanced by their ability to form complexes with humic and fulvic acids, carbonates, hydroxides, and phosphates. Based on the surface water and sediment sample results obtained in this remedial investigation, it appears that several inorganic chemicals are migrating to surface waters at the site, and that the geochemical processes in the surface waters allow for these contaminants to both remain in the water column and sorb to sediments.

8.1.3 SOIL MIGRATION

Contaminants present in surface and subsurface soils may leach to the underlying aquifer. Many factors influence the rate of contaminant movement through soils. These include the physical/chemical properties of the contaminants (e.g., solubility, density, viscosity, K_{oc} , K_{ow}), and the physical/chemical properties of the environment (e.g., rainfall percolation rate, soil permeability, porosity, particle size distribution, organic carbon content). Because all these factors can affect the rate of contaminant movement through soils, it is very difficult to predict such movement. However, based on the data collected in this remedial investigation some gross generalizations of this movement can be made.

Sorption of the chemical to soil particles is the only significant hindrance of contaminant migration in soils at the TP Site. If it were not for sorption, rainfall recharge and soil permeability at this site are high enough such that all the contaminants of concern would readily move through the soils. This is demonstrated by the movement of the volatile organic chemicals and some of the semi-volatile organic chemicals (i.e., the phenols, naphthalenes, dichlorobenzenes, BHC isomers, dibenzofuran, carbazole, and phenanthrene) through the soils. Sorption of these contaminants is relatively small at this site, as indicated by their low K_d values, and thus they have been observed at significant concentrations and/or over significant areas in groundwater. The rest of the semi-volatile organic contaminants of concern, however, have much higher K_d values and even though they have been observed in the soils at significant concentrations, they have not been observed as extensively in groundwater as those with lower K_d values. Sorption of these contaminants of concern to the soils at the site has apparently prevented significant migration into groundwater.

Except for barium (and possibly aluminum, vanadium, and cyanide), the inorganic contaminants of concern also have high K_d values, and thus, these contaminants will also readily sorb to soil particles at the site. However, the observance of some of these inorganic contaminants in groundwater at significant concentrations indicates that the abundance of these contaminants in soil may be too high for

complete sorption to occur. The concentrations of the inorganics in the soils is apparently high enough such that a significant amount of this inorganic contamination can still leach into groundwater. Except for barium (and possibly vanadium, aluminum, and cyanide), movement of the inorganic contaminants of concern in the soils at this site, however, is expected to be very slow due to their high propensity for sorption.

8.1.4 GROUNDWATER MIGRATION

Many factors influence the rate of contaminant movement in an aquifer system. These include the physical/chemical properties of the contaminants (e.g., solubility, density, viscosity, etc.), and the physical/chemical properties of the environment (e.g., soil permeability, porosity, bulk density, particle size distribution, extent and connectivity of fractures, etc.). Because all these factors can affect the rate of contaminant movement through aquifers, it is very difficult to predict such movement. However, based on the data collected in this RI, some gross approximations of this movement can be made.

Once the contaminants of concern reach groundwater, they will generally move as groundwater moves, through the process of advection. However, the process of dispersion will also cause the contaminants to spread both horizontally and vertically. Dispersion generally causes contaminants to migrate (spread) 10 to 20 percent further than migration created by advection alone. Counteractive to the advection and dispersion processes, however, is the process of sorption which will retard the movement of the contaminants. Sorption of contaminants is generally described by their distribution coefficients (K_d). The distribution coefficient can be expressed as:

$$K_{\text{d}} \hspace{0.5cm} = \hspace{0.5cm} \begin{array}{c} \text{mass of contaminant on the solid phase per mass of solid phase} \\ \text{concentration of solute in solution} \end{array}$$

Estimates of the distribution coefficients for the contaminants of concern at the site are presented in Table 8-1. As indicated in this table, the majority of the inorganic contaminants of concern and some of the semi-volatile organic contaminants of concern generally have high K_d values, and thus, these contaminants will readily sorb to soil particles at the site and are essentially immobile. The volatile organic contaminants of concern, some of the semi-volatile organic contaminants of concern, barium, and possibly a few other inorganic contaminants of concern, however, generally have lower K_d values, and thus will not sorb to soil particles as readily as the other contaminants of concern. These contaminants are therefore considered to be mobile, and will generally move as groundwater moves, only at reduced velocities.

To evaluate the potential impacts of the processes described above on contaminant migration in the aquifer system at the TP Site, a groundwater flow and transport model was developed and used to simulate movement of some of the contaminants of concern in groundwater at the site. The development and simulation results of this model are described in detail in **Appendix F**.

The results of groundwater flow modeling indicate that the highly mobile contaminants (i.e., those with a K_d value less than 1 ml/g) could have moved a significant distance from their source in the 78 years since operations began at the coke plant facility, and may have even reached and discharged into Chattanooga Creek. In addition, some of the highly mobile contaminants could have discharged into the Northwest Tributary or the Northeast Tributary. Migration of the lesser mobile contaminants (i.e., those with a K_d value greater than 1 ml/g) in groundwater, however, has likely been limited primarily to the area south of Hamill Road, with some of the lesser mobile contaminants (i.e., those with a K_d value greater than 10 ml/g) not having moved any significant distance from the source areas, due to the high rate of sorption of these contaminants.

8.2 <u>CONTAMINANT PERSISTENCE</u>

Persistence is the measure of how long a chemical will exist in the environment before it degrades or transforms, either chemically or biologically, into some other chemical. Some of the factors which affect the persistence of a chemical include the state of the chemical, the availability of the chemical, exposure to sunlight, oxygen availability, the types and quantities of microorganisms present, availability of nutrients, temperature, pH, as well as the presence of other chemicals which may inhibit or enhance degradation. Usually, persistence is expressed in terms of a chemical half-life and can be on the order of days, weeks, or years.

Because of the many complex factors which may affect persistence, the actual rate of chemical degradation is very difficult to predict for a given chemical at a given site, especially without the benefit of any degradation data collected from site-specific field studies. However, a qualitative evaluation of the potential for degradation of a chemical can be made based on the results of laboratory and/or field studies conducted previously at other locations. Such a qualitative evaluation was conducted for the contaminants of concern detected at the TP Site, and the results are summarized in **Table 8-2.** In this table, the degradation potential for each of the contaminants of concern is indicated for the following three environmental media categories:

- <u>Atmospheric Degradation</u> A chemical released to the atmosphere may degrade by such processes as photolysis and/or reactions with the hydroxyl radical, ozone, or other chemicals present
- Aquatic Degradation A chemical released to fresh, marine, or estuarine surface waters may degrade by such processes as photolysis, hydrolysis, oxidation, and/or biodegradation

TABLE 8-2

ESTIMATED DEGRADATION POTENTIAL OF THE CONTAMINANTS OF CONCERN¹ TENNESSEE PRODUCTS SITE CHATTANOOGA, TENNESSEE

Contaminant	Atmospheric	Aquatic	Terrestrial
of	Degradation	Degradation	Degradation
Concern	Potential	Potential	Potential
<u>Inorganics</u>			
Arsenic	Low	Low	Low
Aluminum	Low	Low	Low
Barium	Low	Low	Low
Beryllium	Low	Low	Low
Cadmium	Low	Low	Low
Iron	Low	Low	Low
Manganese	Low	Low	Low
Nickel	Low	Low	Low
Vanadium	Low	Low	Low
Cyanide	Low/Moderate	Low/Moderate	Low/Moderate
<u>VOCs</u>			
Acetone	High	High	High
Benzene	High	High	High
Carbon Tetrachloride	Low	Low/Moderate	Low/Moderate
Chlorobenzene	High	Moderate	Moderate
Chloroform	Moderate	Low/Moderate	Low/Moderate

TABLE 8-2 (cont.)

ESTIMATED DEGRADATION POTENTIAL OF THE CONTAMINANTS OF CONCERN¹ TENNESSEE PRODUCTS SITE CHATTANOOGA, TENNESSEE

Contaminant of	Atmospheric Degradation	Aquatic Degradation	Terrestrial	
Concern	Potential	Potential	Degradation Potential	
1,2-Dichloroethane	Moderate	Low/Moderate	Low/Moderate	
Ethylbenzene	High	High	Moderate	
Methyl Butyl Ketone	High	High	High	
Tetrachloroethene	Moderate	Low/Moderate	Low/Moderate	
Гoluene	High	High	High	
1,1,1-Trichloroethane	Low	Low/Moderate	Low/Moderate	
Trichloroethene	Moderate	Low/Moderate	Low/Moderate	
<u>SVOCs</u>				
Benzo(a)anthracene	High	Low/Moderate	Low/Moderate	
Benzo(b &/or k)fluoranthene	nzo(b &/or k)fluoranthene High		Low/Moderate	
Benzo-a-pyrene	High	Low/Moderate	Low/Moderate	
Bis(2-ethylhexyl)phthalate	Low	High	Moderate/High	
Carbazole	High	High	High	
Dibenzo(a,h)anthracene	High	Low/Moderate	Low/Moderate	
Dibenzofuran	High	Moderate	Moderate	
1,4-Dichlorobenzene	Moderate/High	Low/Moderate	Low/Moderate	
2,4-Dimethylphenol	High	High	High	
Indeno(1,2,3-cd)pyrene	High	Low/Moderate	Low/Moderate	

TABLE 8-2 (cont.)

ESTIMATED DEGRADATION POTENTIAL OF THE CONTAMINANTS OF CONCERN¹ TENNESSEE PRODUCTS SITE CHATTANOOGA, TENNESSEE

Contaminant	Atmospheric	Aquatic	Terrestrial
of	Degradation	Degradation	Degradation
Concern	Potential	Potential	Potential
2-Methylnaphthalene	High	High	Moderate/High
2-Methylphenol	High	High	High
(3-and/or 4-)Methylphenol	High	High	High
Naphthalene	High	High	High
Phenanthrene	High	Moderate	Moderate
Pesticides/PCBs			
Alpha-BHC	Low	Low/Moderate	Low/Moderate
Beta-BHC	Low	Low/Moderate	Low/Moderate
Delta-BHC	Low	Low/Moderate	Low/Moderate
Dieldrin	Low	Low	Low
PCB-1248	Low/Moderate	Low	Low

¹Qualitative Evaluations Made Based on Information Obtained from the Following Sources:

- 1) U.S. Department of Health and Human Services Toxicological Profiles
- 2) Fate and Exposure Data For Organic Chemicals, (Howard, 1989)
- 3) Hazardous Substance Data Bank maintained by the National Library of Medicine in Bethesda, Maryland

• <u>Terrestrial Degradation</u> - A chemical released to soil or groundwater may degrade by such processes as hydrolysis, oxidation, and/or biodegradation

As indicated in Table 8-2, of all the contaminants of concern at the TP Site, the metals have the least potential to degrade in all media and therefore will likely persist the longest at the site. In fact, these contaminants, under ordinary conditions, will likely persist indefinitely (for all practicable purposes). Other chemicals which also have low degradation potential include the pesticides and PCBs. The contaminants of concern that have the greatest potential for degradation include the BTEX chemicals (benzene, toluene, and ethylbenzene), phenols, acetone, methyl butyl ketone, and the lower molecular weight PAHs (i.e., naphthalene, 2-methylnaphthalene, and carbazole). All the other contaminants of concern generally have low to moderate potentials for degradation, unless released to the atmosphere, in which case all the PAHs generally have a high potential for degradation.